CAREER: Ferroelectric Multilayers, Superlattices, and Compositionally Graded Films
DMR-0132918

PI: S. Pamir Alpay
Department of Materials Science and Engineering, University of Connecticut

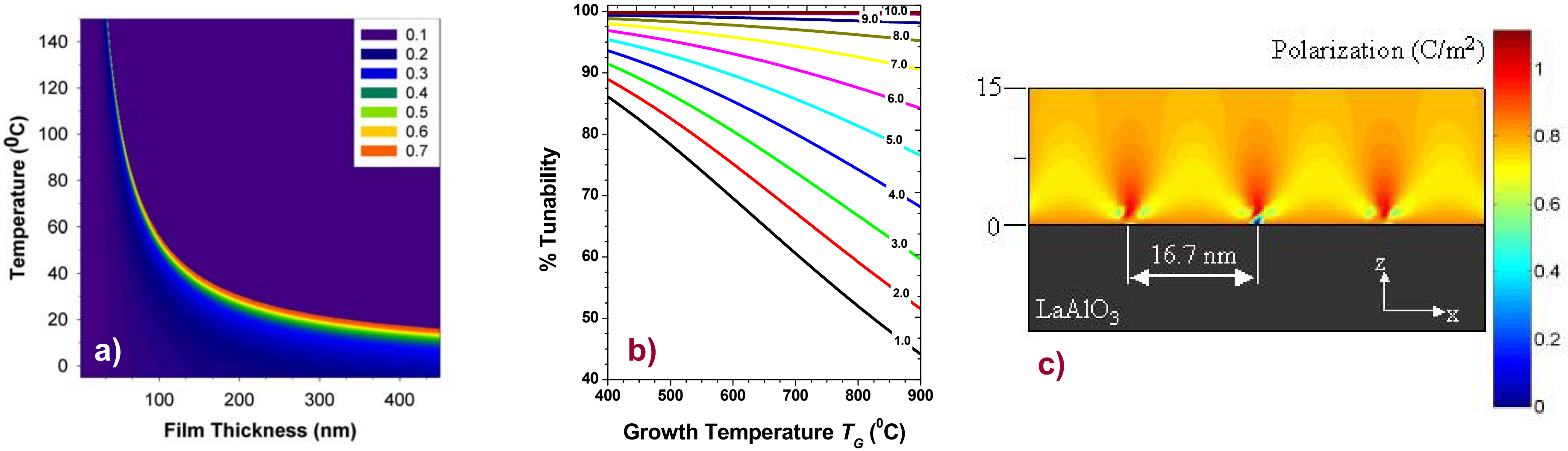

Figure 1. a) Contour map of the pyroelectric response (μC cm^{-2} K^{-1}) of $Ba_{0.6}Sr_{0.4}TiO_3$ thin film grown on $LaAlO_3$ substrate at different operating temperatures and film thickness, b) The variation in the dielectric constant with applied voltage (tunability) for $Ba_{0.5}Sr_{0.5}TiO_3$ thin film as a function of growth temperature and thermal expansion mismatch, c) The calculated effect of crystalline defects (dislocations) on the polarization distribution in $PbTiO_3$ thin film (15 nm thickness) grown on $LaAlO_3$ substrate.

Research: Ferroelectric films are used in infrared (IR) detection (night vision technology). In a contour map, **Fig 1a,** we show predictions of the IR sensitivity of a ferroelectric film as a function of film thickness and operating temperature. When integrated into the micro-circuitry, internal stresses in the film strongly affect the IR response. Enhanced IR properties can be tailored using such maps. The dielectric constant of ferroelectric materials can be altered via an externally applied voltage. This property is called tunability and is used in microwave devices and wireless communication systems. In **Fig 1b,** the tunability of a ferroelectric film is plotted as a function of growth temperature and, parametrically with thermal expansion mismatch between the film and the substrate. Such graphs can be used to improve film properties for a tunable applications. Linear crystalline defects, dislocations, form naturally to relieve internal stresses in thin films. In ferroelectrics, the presence of dislocations creates an inhomogeneous distribution of polarization. We now know that this inhomogeneous variation of polarization due to defects results in internal potentials that degrade electrical properties of ferroelectric films. Our results, shown in **Fig 1c**, show that the density of such defects should be minimized for better device performance.

This CAREER project focuses on the engineering of artificially layered ferroelectric superlattices and compositionally graded ferroelectric films with enhanced properties through spatial variations in internal stresses, film composition, and microstructure. Making use of the unique intrinsic characteristics of ferroelectric materials and introducing compositional and internal stress gradients, exceptional and unusual electrical and electromechanical properties can be obtained which are not possible for bulk ferroelectrics and ferroelectric thin films. Our work anticipates broad classes of entirely new electromagnetic devices: transpacitors, transductors, and transponents. These materials are usually high energy-density materials that can be configured to store and release energy (electrical, magnetic, and mechanical) in well regulated manners, making them highly useful as sensors and actuators. Unlike passive/homogeneous ferroics; transpacitors, transductors, translastics, and other transponent devices (formed from non-homogeneous ferroics) are active devices with potential applications in a multitude of high-sensitivity, high-energy-products: sensors, actuators, and other energy storage and metering devices. Until this present work, there has not been any attempt to undertake a general analysis of non-homogeneous ferroics enabling predictive capabilities for new transponent configurations. Overall, we have published 15 journal articles and 5 refereed conference proceedings. The PI has also submitted a book tentatively entitled "*Graded Ferroelectrics, Transpacitors, and Transponent Devices*" as a part of the Functional Thin Film Materials series to be published by Springer Verlag. The editors selected the topic as it pertains to the creation of a family of totally new devices.

In the third year of the program, we have concentrated on the effect of internal stresses and inhomogeneities in the polarization and their effect on the ferroelectric properties. Some of the relevant conclusions are illustrated in **Figure 1.**

Ferroelectric films are used as active elements in infrared detection (night vision technology). In **Figure 1a**, we show a contour map that may be used to predict the IR sensitivity of a ferroelectric film as a function of film thickness and operating temperature. When integrated into the micro-circuitry, internal stresses in the film strongly affect the IR response. Enhanced IR properties can be tailored using such maps.

The dielectric constant of ferroelectric materials can be tuned via an externally applied voltage. This property is called tunability (relative variation of the dielectric constant with field) and is being used in microwave devices and wireless communication systems. We plot the tunability of a ferroelectric film is a function of growth temperature and the thermal expansion mismatch between the film and the substrate in **Figure 1b**. Such graphs can be used to improve film properties for a tunable applications by optimizing thermal stresses due to thermal expansion mismatch between the film and the substrate.

Linear crystalline defects, dislocations, form naturally to relieve internal stresses in thin films. Dislocations are equilibrium defects. The linear dislocation density and spacing depends on the lattice mismatch at the film deposition temperature and the film thickness. The linear spacing of dislocations for a (001) $PbTiO_3$ thin film (15 nm thick) grown on (001) $LaAlO_3$ substrate is 16.7 nm, calculated from classical thermodynamic analysis of Matthews and Blakeslee. In ferroelectrics, the presence of dislocations creates an inhomogeneous distribution of polarization. Associated with a dislocation there is a non-linear stress field that couples with the polarization through the electrostriction. Depending on the stresses, around the dislocation there are regions with improved polarization and regions with almost no polarization (near the core), **Figure 1c**. We now know that this inhomogeneous distribution of polarization due to defects results in internal potentials that degrade electrical properties of ferroelectric films. Our results show that the density of such defects should be minimized for better device performance.

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Education:

During the past three years, 6 undergraduate students (Mr. Dean Halter, Mr. Scott Virkler, Mr. Michael White, Ms. Sofia Iddir, Ms. Elisabeth Jordan, and Ms. Zoe Weber) and 5 graduate students (Mr. G. Akcay, Dr. (Mr.) Z.-G. Ban, A. Sharma, Mr. I.B. Misirlioglu, and Mr. S. Zhong) contributed to this program.

Dr. Ban received his Ph.D. in 2003 and is presently a post-doc at Argonne National Labs. Mr. Sharma graduated with an M.S. degree in April 2004 and is pursuing a career in business management.

Graduate students presented their work at international conferences (8 invited, 18 contributed presentations).

Outreach:

A popular science web site on the science and technology of thin film materials was developed and uploaded thanks to the efforts of Mr. Halter, Mr. White, Mr. Virkler, and Ms. Weber. They have worked not only on the design of the web pages but on the content as well.